

A Parameterization of Collisions in the Boltzmann Equation by a Rotation Matrix and Boltzmann Collision Integral in Discrete Models of Gas Mixtures

Vladimir L. Saveliev

*Institute of Ionosphere, Kamenskoe Plato, Almaty, 480020, Kazakhstan;
UMR 6614/CORIA/CNRS University of Rouen, 76821 Mont-Saint-Aignan, cedex France*

I. INTRODUCTION

Applications of the group theory constructions remains not broadly used yet in the kinetic theory, as it deserves to be^[1,2]. In the paper, the new opportunities and advantages that the parameterization of two-particle collisions by a matrix from the group of rotations can provide are shown. Usually, to construct the collision integral in the Boltzmann kinetic equation a collision of two particles is determined by setting a direction ($\mathbf{n}, n^2 = 1$) of the relative velocity vector of the particles after the collision^[3].

$$\mathbf{v}' = \frac{m\mathbf{v} + \mathbf{u} + |\mathbf{v} - \mathbf{u}|\mathbf{n}}{1 + m}; \quad \mathbf{u}' = \frac{m\mathbf{v} + \mathbf{u} - m|\mathbf{v} - \mathbf{u}|\mathbf{n}}{1 + m}; \quad \text{where } m = \frac{m_1}{m_2}, \quad \mathbf{v} = \mathbf{v} - \mathbf{u}; \quad (1)$$

In the paper we offer to construct the collision integral using a parameterization of a scattering by a rotation matrix $\hat{R} \in O_3$ which is determined by Euler's angles φ, θ, ψ ^[4].

In this case, the transformation of the velocities due to a collision in contrast to case (1), becomes a linear one:

$$\mathbf{v}' = \frac{m\mathbf{v} + \mathbf{u} + \hat{R}(\mathbf{v} - \mathbf{u})}{1 + m}, \quad \mathbf{u}' = \frac{m\mathbf{v} + \mathbf{u} - m\hat{R}(\mathbf{v} - \mathbf{u})}{1 + m}; \quad (2)$$

and is representing by scattering matrix \hat{S} a partitioned matrix (2×2 cells). The size of each cell obviously is (3×3):

$$\xi' = \hat{S}\xi, \quad \xi = \begin{pmatrix} \mathbf{v} \\ \mathbf{u} \end{pmatrix}, \quad \hat{S} = \begin{pmatrix} \frac{m + \hat{R}}{1 + m} & \frac{1 - \hat{R}}{1 + m} \\ \frac{m(1 - \hat{R})}{1 + m} & \frac{1 + m\hat{R}}{1 + m} \end{pmatrix}; \quad (3)$$

Also in contrast to (1), that linear transformation due to $|\det \hat{S}| = 1$ provides the equality of velocity volumes

$$d\mathbf{v}d\mathbf{u} = d\mathbf{v}'d\mathbf{u}' \quad (4).$$

The matrixes $\hat{S}(\hat{R}), \hat{R} \in O_3$ constitute a group: $\hat{S}(\hat{R}_1) \cdot \hat{S}(\hat{R}_2) = \hat{S}(\hat{R}_1 \cdot \hat{R}_2), \hat{S}^{-1}(\hat{R}) = \hat{S}(\hat{R}^{-1})$.

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.				
1. REPORT DATE (DD-MM-YYYY) 09-07-2000		2. REPORT TYPE Conference Proceedings		3. DATES COVERED (FROM - TO) 09-07-2000 to 14-07-2000
4. TITLE AND SUBTITLE A Parameterization of Collisions in the Boltzmann Equation by a Rotation Matrix and Boltzmann Collision Integral in Discrete Models of Gas Mixtures Unclassified			5a. CONTRACT NUMBER	
			5b. GRANT NUMBER	
			5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Saveliev, Vladimir L. ;			5d. PROJECT NUMBER	
			5e. TASK NUMBER	
			5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME AND ADDRESS Institute of ionosphere Kamenskoe Plato Almaty 480020, Kazakhstanxxxxx			8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME AND ADDRESS AOARD Unit 45002 APO AP, 96337-5002			10. SPONSOR/MONITOR'S ACRONYM(S)	
			11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT APUBLIC RELEASE				
13. SUPPLEMENTARY NOTES See Also ADM001341, Rarefied Gas Dynamics (RGD) 22nd International Symposium held in Sydney, Australia, 9-14 July 2000.				
14. ABSTRACT Applications of the group theory constructions remains not broadly used yet in the kinetic theory, as it deserves to be[1,2]. In the paper, the new opportunities and advantages that the parameterization of two-particle collisions by a matrix from the group of rotations can provide are shown.				
15. SUBJECT TERMS				
16. SECURITY CLASSIFICATION OF:		17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19. NAME OF RESPONSIBLE PERSON
		Public Release	8	Fenster, Lynn lfenster@dtic.mil
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified	19b. TELEPHONE NUMBER International Area Code Area Code Telephone Number 703767-9007 DSN 427-9007	
				Standard Form 298 (Rev. 8-98) Prescribed by ANSI Std Z39.18

II. THE COLLISION INTEGRAL

To write the collision integral the integration over relative velocity directions should be replaced $\int \frac{d\Omega_n}{4\pi} \rightarrow \int \frac{d\hat{R}}{16\pi^2}$ with integration on the invariant ($d\hat{R} = d\hat{R}_0 \hat{R} = d\hat{R} \hat{R}_0 = d\hat{R}^{-1}$) measure^[4] over the group O_3 : $d\hat{R} = d\psi d\varphi \sin \theta d\theta$, $0 \leq \psi, \theta, \varphi < 2\pi$, $\int d\hat{R} = 16\pi^2$. As a result, we get the collision integral written in an explicitly invariant and simple form:

$$I(f, \Psi) = I(F) = \int b(\mathbf{v}, \hat{R}) [f(\mathbf{v}') \Psi(\mathbf{u}') - f(\mathbf{v}) \Psi(\mathbf{u})] \frac{d\hat{R}}{4\pi} d\mathbf{u} = \int b(\mathbf{v}, \hat{R}) [F(\hat{S}(\hat{R})\xi) - F(\xi)] \frac{d\hat{R}}{4\pi} d\mathbf{u}, \quad (5)$$

where $b(\mathbf{v}, \hat{R}) = v \sigma_\theta(\mathbf{v}, \mu(\hat{R}))$ is a scattering indicatrix, $\mu(\hat{R}) = \frac{\mathbf{v} \cdot \hat{R} \mathbf{v}}{v^2}$ — cosine of the scattering angle, $F(\xi) = f \circ \Psi(\xi) = f(\mathbf{v}) \Psi(\mathbf{u})$ is a two-particle velocity distribution function. Taking into consideration that $\delta(\mathbf{v}' - \mathbf{v}_0) \delta(\mathbf{u}' - \mathbf{u}_0) = \delta(\hat{S}\xi - \xi_0) = \delta(\xi - \hat{S}(\hat{R}^{-1})\xi_0)$ we have decomposition formula for δ -functions:

$$I(\delta(\mathbf{v} - \mathbf{v}_0), \delta(\mathbf{u} - \mathbf{u}_0)) = I(\delta(\xi - \xi_0)) = \int \frac{d\hat{R}}{4\pi} b(\mathbf{v}_0, \hat{R}) [\delta(\mathbf{v} - \mathbf{v}') - \delta(\mathbf{v} - \mathbf{v}_0)], \quad (6)$$

And similar for Maxwellians:

$$I(f_M(\mathbf{v} - \mathbf{v}_0), \Psi_M(\mathbf{u} - \mathbf{u}_0)) = \int \frac{d\hat{R}}{4\pi} [b_T(\mathbf{v}, \mathbf{u}'_0, \hat{R}) f_M(\mathbf{v} - \mathbf{v}'_0) - b_T(\mathbf{v}, \mathbf{u}_0, \hat{R}) f_M(\mathbf{v} - \mathbf{v}_0)], \quad (7)$$

where $b_T(\mathbf{v}, \mathbf{u}_0, \hat{R}) = \int b(\mathbf{v}, \hat{R}) \Psi_M(\mathbf{u} - \mathbf{u}_0) d\mathbf{u}$.

At the zero temperature limit we obtain the asymptotic equality similar to property (6):

$$I(f_M(\mathbf{v} - \mathbf{v}_0) \Psi_M(\mathbf{u} - \mathbf{u}_0))_{T \rightarrow 0} = \int \frac{d\hat{R}}{4\pi} b(\mathbf{v}_0, \hat{R}) [f_M(\mathbf{v} - \mathbf{v}'_0) - f_M(\mathbf{v} - \mathbf{v}_0)] + O(T), \quad (8)$$

For Maxwell's molecules (and asymptotically in the limit $T \rightarrow 0$ in the general case) those two decompositions coincide. In the case of the Maxwell molecules the indicatrix b does not depend on a velocity and consequently equality (8) is satisfied at all temperatures and is a corollary of the invariance of the collision operator with constant collision frequency with respect to Gauss transformation^[11]:

$$e^{\frac{kT}{2m_1} \nabla_v^2} I(f, \Psi) = I \left(e^{\frac{kT}{2m_1} \nabla_v^2} f, e^{\frac{kT}{2m_2} \nabla_u^2} \Psi \right), \quad (9)$$

where

$$e^{\frac{kT}{2m} \nabla_v^2} f(\mathbf{v}) = \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \int d\mathbf{v}' e^{-\frac{m(\mathbf{v}-\mathbf{v}')^2}{2kT}} f(\mathbf{v}'), \quad \nabla_v^2 = \left(\frac{\partial}{\partial \mathbf{v}} \right)^2, \quad \nabla_u^2 = \left(\frac{\partial}{\partial \mathbf{u}} \right)^2.$$

III. THE COLLISION INTEGRAL FOR DISCRETE MODELS

The form of collision operator obtained above is very useful in an application to the discrete models^[5-9]. An explicit expression for the collision integral suitable for the discrete models can be constructed, if we replace in collision integral (5) the averaging over rotations from group of rotations O_3 with an averaging over its discrete subgroup

$$\text{consisting of finite number } K \text{ elements } \left(\int \frac{d\hat{R}}{16\pi^2} \rightarrow \frac{1}{K} \sum_{k=1}^K \hat{R}_k \right); \quad (10)$$

$$I_d(f, \Psi) = \frac{4\pi}{K} \int d\mathbf{u} \sum_{k=1}^K b(\mathbf{v}, \hat{R}_k) [f(\mathbf{v}') \Psi(\mathbf{u}') - f(\mathbf{v}) \Psi(\mathbf{u})] = \frac{4\pi}{K} \int d\mathbf{u} \sum_{k=1}^K b(\mathbf{v}, \hat{R}_k) [F(\hat{S}(\hat{R}_k)\xi) - F(\xi)]$$

The expressions given by formulae (6) and (8) in this case are reduced to the finite sums:

$$I_d(\delta(\mathbf{v} - \mathbf{v}_0) \delta(\mathbf{u} - \mathbf{u}_0)) = \frac{4\pi}{K} \sum_{k=1}^K b(\mathbf{v}_0, \hat{R}_k) [\delta(\mathbf{v} - \mathbf{v}_0') - \delta(\mathbf{v} - \mathbf{v}_0)], \quad (11)$$

and

$$I_d(f_M(\mathbf{v} - \mathbf{v}_0) \Psi_M(\mathbf{u} - \mathbf{u}_0))_{T \rightarrow 0} = \frac{4\pi}{K} \sum_{k=1}^K b(\mathbf{v}_0, \hat{R}_k) [f_M(\mathbf{v} - \mathbf{v}_0') - f_M(\mathbf{v} - \mathbf{v}_0)] + O(T). \quad (12)$$

Formulae (11) and (12) give an explicit representation of the collision terms in the set of equations for discrete gas models, which can be obtained from the initial Boltzmann kinetic equations after a substitution of distribution functions in them in a form of an expansion on delta-functions or on Maxwell velocity clusters.

IV. SCATTERING VARIABLES AND AN INVARIANT ENSEMBLE OF PAIRS OF DISCRETE VELOCITIES.

A state of a pair of colliding particles in the kinetic theory is usually characterized by particle velocities \mathbf{v} and \mathbf{u} . The state also can be uniquely characterized by other variables that are linear combinations of the velocities \mathbf{v} and \mathbf{u} and which transform in collisions much simpler. It is convenient to choose variables \mathbf{p} and \mathbf{w} as such scattering variables. The variable \mathbf{w} is a center of masses velocity, and \mathbf{p} is a momentum of the first particle in a center of masses frame of reference. Formulae of transformation from a variables \mathbf{v} , \mathbf{u} to variables \mathbf{p} , \mathbf{w} and back look as follows:

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{w} \end{pmatrix} = \hat{A} \cdot \begin{pmatrix} \mathbf{v} \\ \mathbf{u} \end{pmatrix}, \quad \hat{A} = \frac{m_1 m_2}{m_1 + m_2} \begin{pmatrix} 1 & -1 \\ m_2^{-1} & m_1^{-1} \end{pmatrix}; \quad \begin{pmatrix} \mathbf{v} \\ \mathbf{u} \end{pmatrix} = \hat{A}^{-1} \cdot \begin{pmatrix} \mathbf{p} \\ \mathbf{w} \end{pmatrix}, \quad \hat{A}^{-1} = \begin{pmatrix} m_1^{-1} & 1 \\ -m_2^{-1} & 1 \end{pmatrix}. \quad (13)$$

The matrix of scattering in the variables \mathbf{p} , \mathbf{w} becomes cell-diagonal. In fact, a velocity of a center of masses after collision does not change ($\mathbf{w}' = \mathbf{w}$) and the momentum \mathbf{p} is rotating by a rotation matrix \hat{R} , $\mathbf{p}' = \hat{R}\mathbf{p}$. Consequently, the matrix of scattering in these variables has a form:

$$\hat{S}_A = \hat{A} \hat{S} \hat{A}^{-1} = \begin{pmatrix} \hat{R} & 0 \\ 0 & 1 \end{pmatrix}; \quad (14)$$

If we will consider a model of gas in which not all possible scatterings in a pair of colliding particles happen, but only related to rotation matrixes $\hat{R} \in O_3(K) \subset O_3$ from some discrete subgroup $O_3(K)$ containing K elements, it is possible to construct an ensemble of pairs of discrete velocities, that transforms into itself by the collision transformations. There are several ways to construct such ensembles. We consider purely lattice way. In this case the velocity of a center of masses is given by an integer linear combination of the basis vectors of a lattice $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$, and the momentum of the first particle is given by a linear superposition of the vectors $m_0 \mathbf{w}_1, m_0 \mathbf{w}_2, m_0 \mathbf{w}_3$ with integer coefficients. A set of six integer numbers $l_1, l_2, l_3, k_1, k_2, k_3$ will be coordinates of velocity pairs:

$$\begin{aligned} \mathbf{p}(l_1, l_2, l_3) &= l_1 m_0 \mathbf{w}_1 + l_2 m_0 \mathbf{w}_2 + l_3 m_0 \mathbf{w}_3, \\ \mathbf{w}(k_1, k_2, k_3) &= k_1 \mathbf{w}_1 + k_2 \mathbf{w}_2 + k_3 \mathbf{w}_3. \end{aligned} \quad (15)$$

For discrete velocities in accordance to (13) one will have:

$$\begin{aligned} \mathbf{v}_\alpha &= \mathbf{v}_\alpha(l_1, l_2, l_3, k_1, k_2, k_3) = \left(\frac{m_0}{m_\alpha} l_1 + k_1 \right) \mathbf{w}_1 + \left(\frac{m_0}{m_\alpha} l_2 + k_2 \right) \mathbf{w}_2 + \left(\frac{m_0}{m_\alpha} l_3 + k_3 \right) \mathbf{w}_3 \in L_\alpha; \\ \mathbf{u}_\beta &= \mathbf{v}_\beta(-l_1, -l_2, -l_3, k_1, k_2, k_3) \in L_\beta; \quad l_1, l_2, l_3, k_1, k_2, k_3 = 0, \pm 1, \pm 2, \dots; \\ \mathbf{v}'_\alpha &= \left(\frac{m_0}{m_\alpha} l_1 \hat{R} + k_1 \right) \mathbf{w}_1 + \left(\frac{m_0}{m_\alpha} l_2 \hat{R} + k_2 \right) \mathbf{w}_2 + \left(\frac{m_0}{m_\alpha} l_3 \hat{R} + k_3 \right) \mathbf{w}_3, \quad \mathbf{u}'_{0\beta} = \mathbf{v}'_\beta(-l_1, -l_2, -l_3, k_1, k_2, k_3); \end{aligned} \quad (16)$$

The vectors $\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3$ are basic vectors of the Bravais lattice invariant regarding a discrete subgroup of rotations (the point groups),

$$\hat{R} \mathbf{w}_i = \sum_k \mathbf{w}_k T_{ki}(\hat{R}), \quad (17)$$

where $T_{ki}(\hat{R})$ are unimodular matrixes with integer matrix elements. In the theory of crystals^[10,11] known that there are 14 types of the Bravais lattices and 7 point symmetry groups of these lattices: $S_2, C_{2h}, D_{2h}, D_{3h}, D_{4h}, D_{6h}, O_h$ corresponding to 7 syngonies (triclinic, monoclinic, rhombic, trigonal, tetragonal, hexagonal, cubic). These 7 groups have 32 point subgroups. The only group not having a preferential direction and consequently the most appropriate one for our purposes is the O_h group. That is the group of symmetry of a cube (isomorphic to the group of symmetry of an octahedron) is consisting of 48 elements. Its subgroups without a preferential direction are: the group of proper rotations of a cube $O(24)$, the group of symmetry of a tetrahedron $T_d(24)$, the group of proper rotations of a tetrahedron $T(12)$ and the $T_h(24)$ group of proper rotations of a tetrahedron with an inversion added. The number of elements in these groups is indicated in brackets. For plane Bravais lattices there are only 10 point groups of symmetry: C_1, C_2, C_3, C_4, C_6 that are the groups of rotations around axes of the 1-st, 2-nd, 3-rd, 4-th and 6-th order (angles of rotations in the groups are divisible by either $\frac{\pi}{2}$, or $\frac{\pi}{3}$) and the groups D_1, D_2, D_3, D_4, D_6 that are the groups of rotations C_n with a reflection in an axis lying in a plane of the lattice. For a one-dimensional lattice, obviously, there are only two groups. Those are the identical transformation E and the group with a reflection $\{E, -E\}$. The fact of necessity of a rational masses ratio has been discovered and first lattices of discrete velocities for a mixture of gases have been constructed in paper^[8], paper^[9] is devoted to *spurious* invariants in discrete models.

Presenting velocity distribution functions $f_\alpha(\mathbf{v})$ by the expansions on Dirac delta-functions concentrated on the velocities of the discrete sets L_α ,

$$f_\alpha(\mathbf{v}) = \sum_{\mathbf{v}_0 \in L_\alpha} \bar{f}(\mathbf{v}_0) \delta(\mathbf{v} - \mathbf{v}_0), \quad (18)$$

and two-particle distribution functions of a pair of colliding particles of the sorts α and β by the expansions on Dirac delta-functions concentrated on bivectors from the invariant ensembles $L_{\alpha\beta}$,

$$f_{\alpha\beta}(\xi) = \sum_{\xi_0 \in L_{\alpha\beta}} \bar{f}_\alpha(\mathbf{v}_0) \bar{f}_\beta(\mathbf{u}_0) \delta(\mathbf{v} - \mathbf{v}_0) \delta(\mathbf{u} - \mathbf{u}_0), \quad (19)$$

we obtain an analog of the Boltzmann equation for discrete models for gas mixtures of M components in the following explicit form:

$$\frac{\partial \bar{f}_\alpha(\mathbf{v}_0)}{\partial t} + \mathbf{v}_0 \cdot \frac{\partial \bar{f}_\alpha(\mathbf{v}_0)}{\partial \mathbf{r}} = \sum_{\beta} \sum_{\{\mathbf{u}_0 | (\mathbf{v}_0, \mathbf{u}_0) \in L_{\alpha\beta}\}} \frac{4\pi}{K} \sum_{k=1}^K b_{\alpha\beta}(\mathbf{v}, \hat{R}_k) [\bar{f}_\alpha(\mathbf{v}') \bar{f}_\beta(\mathbf{u}') - \bar{f}_\alpha(\mathbf{v}_0) \bar{f}_\beta(\mathbf{u}_0)] \quad (20)$$

$\mathbf{v}_0 \in L_\alpha; \quad \alpha, \beta = 1, \dots, M.$

Where L_α are sets of discrete velocities $\mathbf{v}_{0\alpha}$ for each mixture component depend only on the mass m_α ; $L_{\alpha\beta}$ are sets of colliding pairs $(\mathbf{v}_{0\alpha}, \mathbf{u}_{0\beta})^T \in L_{\alpha\beta}$; M is number of mixture components. The definition $\{\mathbf{u}_0 | (\mathbf{v}_0, \mathbf{u}_0) \in L_{\alpha\beta}\} \equiv L_{\alpha\beta}(\mathbf{v}_0)$ means a set of all \mathbf{u}_0 for which the pair $(\mathbf{v}_0, \mathbf{u}_0)$ with the given \mathbf{v}_0 is contained in the invariant ensemble $L_{\alpha\beta}$.

V. EXAMPLE OF DISCRETE VELOCITY MODEL CONSTRUCTED ON THE GROUP OF SYMMETRY OF A CUBE O_h

Rotation on angle B around axis \mathbf{B} is given by formula:

$$\exp \hat{B} = \frac{1 - \cos B}{B^2} \hat{B}^2 + \frac{\sin B}{B} \hat{B} + 1 \quad (21)$$

where the operator (matrix) \hat{B} is defined by the following expression:

$$\hat{B} \stackrel{df}{=} \mathbf{B} \times, \quad \hat{B} \mathbf{v} \stackrel{df}{=} \mathbf{B} \times \mathbf{v}; \quad (22)$$

We will describe nontrivial rotations from the group O by vectors $\mathbf{B}_1, \dots, \mathbf{B}_{23}$. Rotation on the zero angle (trivial rotation) is the unity transformation \hat{E} :

$$\mathbf{B}_0 = 0, \quad \exp(\hat{B}_0) = \hat{E} \quad (23)$$

Symmetry of a cube includes three fourth order axes coming through centers of opposite faces of a cube (9 nontrivial rotations):

$$\{\mathbf{B}\}_{1,\dots,9} = \pm \frac{\pi}{2}(1,0,0), \pm \frac{\pi}{2}(0,1,0), \pm \frac{\pi}{2}(0,0,1), \pi(1,0,0), \pi(0,1,0), \pi(0,0,1), \quad (24)$$

four third order axes coming through opposite corners of the cube (8 nontrivial rotations):

$$\{\mathbf{B}\}_{10,\dots,17} = \pm \frac{2\pi}{3} \left(\pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}} \right), \quad (25)$$

and six second order axes coming through centers of opposite edges of the cube (6 nontrivial rotations):

$$\{\mathbf{B}\}_{18,\dots,23} = \pi \left(0, \frac{\pm 1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right), \pi \left(\frac{1}{\sqrt{2}}, 0, \frac{\pm 1}{\sqrt{2}} \right), \pi \left(\frac{\pm 1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right), \quad (26)$$

One can obtain the group of all transformations of symmetry of a cube \mathbf{O}_h by adding the inversion transformation $(-\hat{E})$ to the group \mathbf{O} . All 48 elements of the group can be written making use of definitions (21)—(26) as

$$\{\hat{R}\}_{\mathbf{O}_h} = \left\{ \pm \exp(\hat{B}_n), n = 0, 1, \dots, 23 \right\}. \quad (27)$$

There are three Bravais lattices (cubic system), which are invariant under transformations from group \mathbf{O}_h . The first one is the simple cubic lattice $\mathbf{\Gamma}_c$. Sites of that lattice are situated in corners of identical cubes:

$$\mathbf{w}(k_1, k_2, k_3) = k_1 \mathbf{w}_1 + k_2 \mathbf{w}_2 + k_3 \mathbf{w}_3, \quad k_1, k_2, k_3 = 0, \pm 1, \pm 2 : : ,$$

where vectors of elementary periods are

$$\mathbf{w}_1 = (1, 0, 0), \quad \mathbf{w}_2 = (0, 1, 0), \quad \mathbf{w}_3 = (0, 0, 1). \quad (28)$$

The body centered cubic lattice $\mathbf{\Gamma}_c^v$ is a lattice with sites, which are situated in vertices of cubes, and in its centers. Vectors of elementary periods of the lattice are three vectors from a center of the cube to any three vertices. One of the possible variants is:

$$\mathbf{w}_1 = \left(\frac{-1}{2}, \frac{1}{2}, \frac{1}{2} \right), \quad \mathbf{w}_2 = \left(\frac{1}{2}, \frac{-1}{2}, \frac{1}{2} \right), \quad \mathbf{w}_3 = \left(\frac{1}{2}, \frac{1}{2}, \frac{-1}{2} \right). \quad (29)$$

A face-centered lattice $\mathbf{\Gamma}_c^f$ is a lattice with sites situated in corners of cubes and in centers of faces. Vectors of elementary periods of the lattice are three vectors from any corner of a cube to centers of three faces. One of the possible variants is:

$$\mathbf{w}_1 = \left(0, \frac{1}{2}, \frac{1}{2} \right), \quad \mathbf{w}_2 = \left(\frac{1}{2}, 0, \frac{1}{2} \right), \quad \mathbf{w}_3 = \left(\frac{1}{2}, \frac{1}{2}, 0 \right) \quad (30)$$

Here we will describe characteristics of discrete velocity models constructed on simple cubic lattice (28). Substituting elementary periods of this lattice (28) to (16) one will have a relevant discrete velocity model. For discrete velocities components we will have the following expressions:

$$\begin{aligned} v_x &= \frac{m_0}{m_1} l_1 + k_1; & v_y &= \frac{m_0}{m_1} l_2 + k_2; & v_z &= \frac{m_0}{m_1} l_3 + k_3; \\ u_x &= -\frac{m_0}{m_2} l_1 + k_1; & u_y &= -\frac{m_0}{m_2} l_2 + k_2; & u_z &= -\frac{m_0}{m_2} l_3 + k_3; \end{aligned} \quad (31)$$

where $k_1, k_2, k_3 = 0, \pm 1, \dots, \pm k_m$; $l_1, l_2, l_3 = 0, \pm 1, \dots, \pm l_m$. It is seen from (31) that discrete velocity sets for components v_x, v_y, v_z are the same independent sets. To have a number of different discrete velocities less then

number of collisions (bivectors from invariant ensemble) $\frac{m_1}{m_0}$ and $\frac{m_2}{m_0}$ should be rational numbers:

$$\frac{m_1}{m_0} = \frac{p_1}{q_1}; \quad \frac{m_2}{m_0} = \frac{p_2}{q_2}; \quad (32)$$

where p_1, p_2, q_3, q_4 are integer numbers and at list the following inequalities should be held

$$2l_m + 1 \geq p_1, p_2; \quad 2k_m + 1 \geq q_1, q_2 \quad (33)$$

To obtain all different discrete velocities of particles with mass $m = \frac{p}{q}$ one should take indexes l and k in the range:

$$\begin{aligned} l &= -l_m, \dots, (-l_m + p); & k &= -k_m, \dots, k_m & \text{and} & & l &= (-l_m + p + 1), \dots, l_m; & k &= (k_m - q), \dots, k_m \\ v_x &= \frac{q}{p} l + k; \end{aligned} \quad (34)$$

Total number of different discrete velocities v_x for particles with mass $m = \frac{p}{q}$ will be:

$$\begin{aligned} N_x \left(\frac{p}{q} \right) &= p(2k_m + 1) + q(2l_m + 1) - pq, & q &\leq 2k_m + 1, \quad p \leq 2l_m + 1 \\ N_x \left(\frac{p}{q} \right) &= (2l_m + 1)(2k_m + 1), & q &> 2k_m + 1 \quad \text{or} \quad p > 2l_m + 1 \end{aligned} \quad (35)$$

For illustration we here consider the specific gas mixture consisting of $Ne(20)$, $NO(30)$ and $Ar(40)$ gases. The relevant discrete model has the following parameters:

$$l_m = k_m = 5; \quad m_0 = 20; \quad p_1 = 1, \quad q_1 = 1; \quad p_2 = 3, \quad q_2 = 2; \quad p_3 = 2, \quad q_3 = 1; \quad (36)$$

For one-dimensional case ($v_y = v_z = 0$) according to (35) the number of different velocities for each gas component of the mixture will be:

$$N\left(\frac{1}{1}\right)=21, \quad N\left(\frac{3}{2}\right)=49, \quad N\left(\frac{2}{1}\right)=31 \quad (37)$$

The number of effective collisions (the number of bevectors from invariant ensemble with nonzero relative velocity, $l_1 \neq 0$) for each two gases of the mixture is

$$N_c = 2l_m \times (2k_m + 1) = 110 \quad (38)$$

and

$$N_c > 2N\left(\frac{1}{1}\right), \quad N\left(\frac{1}{1}\right) + N\left(\frac{3}{2}\right), \quad N\left(\frac{1}{1}\right) + N\left(\frac{2}{1}\right), \quad 2N\left(\frac{3}{2}\right), \quad N\left(\frac{3}{2}\right) + N\left(\frac{2}{1}\right), \quad 2N\left(\frac{2}{1}\right) \quad (39)$$

$$110 > (2 \times 21 = 42), (21 + 49 = 70), (21 + 31 = 52), (2 \times 49 = 98), (49 + 31 = 80), (2 \times 31 = 62)$$

Due to inequalities (39) this discrete model do not has *spurious* invariants.

The two dimensional ($v_z = 0$) model with $l_m = k_m = 3$ has the following characteristics:

$$l_m = k_m = 3; \quad m_0 = 20, \quad p_1 = 1, \quad q_1 = 1; \quad p_2 = 3, \quad q_2 = 2; \quad p_3 = 2, \quad q_3 = 1; \quad (40)$$

$$N\left(\frac{1}{1}\right)=169, \quad N\left(\frac{3}{2}\right)=841, \quad N\left(\frac{2}{1}\right)=361; \quad N_c = [(2l_m + 1)^2 - 1] \times (2k_m + 1)^2 = 2352$$

And calculated in the same way there are characteristics of the full three dimensional discrete model:

$$l_m = k_m = 2, \quad m_0 = 20, \quad p_1 = 1, \quad q_1 = 1; \quad p_2 = 3, \quad q_2 = 2; \quad p_3 = 2, \quad q_3 = 1; \quad (41)$$

$$N\left(\frac{1}{1}\right)=729, \quad N\left(\frac{3}{2}\right)=6859, \quad N\left(\frac{2}{1}\right)=2197; \quad N_c = [(2l_m + 1)^3 - 1] \times (2k_m + 1)^3 = 15500$$

REFERENCES

1. Saveliev, V.L., "Temperature and mass dependence of the Boltzmann linear collision operator from the group theory point of view," J. Math. Phys. **37**, 6139-6151 (1996).
2. Saveliev, V.L., "Group theory description of temperature and mass dependence of linear Boltzmann collision operator." Rarefied Gas Dynamics Volume I. Proceedings of 21st International Symposium on Rarefied Gas Dynamics-98, edited by R.Brun et al., CEPADUES-EDITIONS, Toulouse, 1999, pp.31-37,
3. Landau, L.D., and Lifshitz E.M., Mechanics, 3rd ed. Pergamon, New York, 1976.
4. Vilenkin, N.I., Special functions and theory of group representation, Nauka, Moscow, 1965 (in Russian).
5. Gatignol, R., Theorie Cinetique des Gas a Repartition Discrete de Vitesses, Lect. Notes in Phys., 36, Springer, Berlin, 1975.
6. Sultangazin, U.M., Methods of spherical harmonics and discrete ordinates in the problems of transport kinetic theory, Nauka Kaz SSR, Alma-Ata, 1979 (in Russian).
7. Cabannes, H., The discrete Boltzmann Equation, Lecture Notes, University of California, Berkely, 1980.
8. Bobylev, A.V., and Cercignani C. "Discrete models for mixtures," Rarefied Gas Dynamics Volume I. Proceedings of 21st International Symposium on Rarefied Gas Dynamics-98, edited by R.Brun et al., CEPADUES-EDITIONS, Toulouse, 1999, pp.24-30
9. Bobylev, A.V., Cercignani C. "Discrete velocity models without nonphysical invariants" (submitted to J. Stat. Phys. in April 1999).
10. Petrashen, M.I., and Trifonov E.D., Application of group theory in quantum mechanics, Nauka, Moscow, 1967 (in Russian).
11. Hamermesh, M., Group theory and its application to physical problems, Addison - Wesley publishing company, Inc. Reading, Massachusetts - Palo Alto - London, 1964